

=> b reg
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STRUCTURE FILE UPDATES: 5 NOV 2007 HIGHEST RN 952474-38-3
DICTIONARY FILE UPDATES: 5 NOV 2007 HIGHEST RN 952474-38-3

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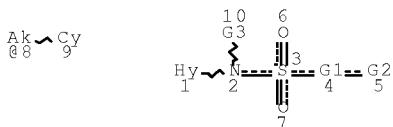
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stnqgen/stndoc/properties.html>

=> d que sta 18
L3 STR



REP G1=(2-3) A
VAR G2=CY/8
VAR G3=H/ME
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E5 C E1 N AT 1

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L6 1217938 SEA FILE=REGISTRY ABB=ON PLU=ON 46.156.1/RID
L8 379 SEA FILE=REGISTRY SUB=L6 SSS FUL L3

100.0% PROCESSED 166426 ITERATIONS 379 ANSWERS
SEARCH TIME: 00.00.03

=> d bib abs hitstr 120 tot
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:n

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FILE 'HCAPLUS' ENTERED AT 11:34:46 ON 06 NOV 2007
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FILE COVERS 1907 - 6 Nov 2007 VOL 147 ISS 20
FILE LAST UPDATED: 5 Nov 2007 (20071105/ED)

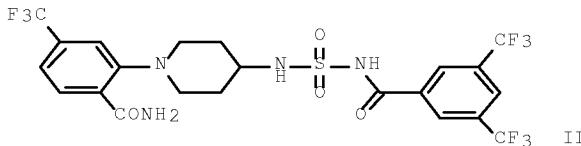
New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d bib abs hitstr 120 tot

L20 ANSWER 1 OF 2 HCPLUS COPYRIGHT 2007 ACS on STN
AN 2003:796680 HCPLUS Full-text
DN 139:307797
TI Preparation of piperazinyl- or piperidinylamine-sulfamic acid amides as inhibitors of steroid sulfatase
IN Lehr, Philipp
PA Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2003082842	A1	20031009	2003WO-EP03214	20030327
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	AU2003226732	A1	20031013	2003AU-0226732	20030327
	EP---1492782	A1	20050105	2003EP-0745281	20030327
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
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	CN---1646509	A	20050727	2003CN-0808336	20030327
	JP2005526812	T	20050908	2003JP-0580309	20030327
	NZ---535617	A	20060428	2003NZ-0535617	20030327
	IN2004CN02142	A	20060303	2004IN-CN02142	20040927
	MX2004PA09453	A	20050125	2004MX-PA09453	20040928
	NO2004004321	A	20041012	2004NO-0004321	20041012
	US2006052393	A1	20060309	2005US-0509259	20050503
	ZA---200407853	A	20060531	2004ZA-0007853	20051213
PRAI	2002GB-0007500	A	20020328		
	2002GB-0025679	A	20021104		
	2003WO-EP03214	W	20030327		
OS	MARPAT 139:307797				
GI					



AB The title compds. R1NR2SO2NHCOR3 [I; NR1R2 = piperazino (wherein the second N atom is substituted by alkoxy carbonyl or aryl) ; or R1 = H and R2 = piperidinyl, attached via a carbon atom of the piperidinyl ring (wherein N is substituted by alkoxy carbonyl or aryl); R3 = aryl, arylalkyl], useful for the manufacture of a medicament in diseases mediated by the action of steroid sulfatase, were prepared E.g., a 5-step synthesis of II (starting from 4-benzylaminopiperidine-1-carboxylic

acid tert-Bu ester and sulfamide), was given. The compds. I show activity in the assay of human steroid sulfatase (rel IC50 in the range of 0.0046 to 350). Pharmaceutical composition comprising the compound I is claimed.

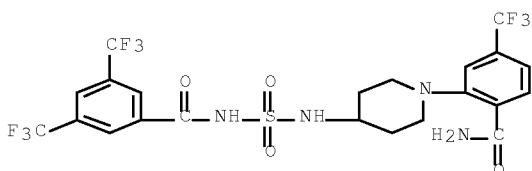
IT 610798-69-1P 610798-74-3P 610798-79-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazinyl- or piperidinylamine-sulfamic acid amides as inhibitors of steroid sulfatase)

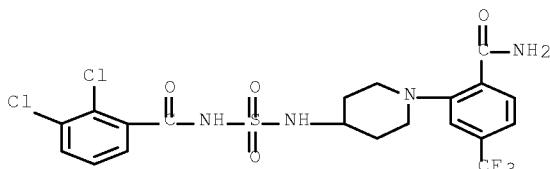
RN 610798-69-1 HCPLUS

CN Benzamide, N-[[[1-[2-(aminocarbonyl)-5-(trifluoromethyl)phenyl]-4-piperidinyl]amino]sulfonyl]-3,5-bis(trifluoromethyl)- (CA INDEX NAME)



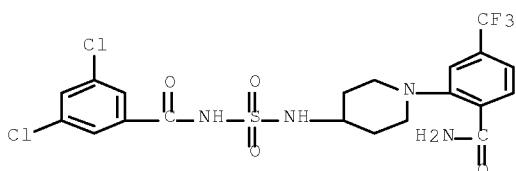
RN 610798-74-8 HCPLUS

CN Benzamide, N-[[[1-[2-(aminocarbonyl)-5-(trifluoromethyl)phenyl]-4-piperidinyl]amino]sulfonyl]-2,3-dichloro- (CA INDEX NAME)



RN 610798-79-3 HCPLUS

CN Benzamide, N-[[[1-[2-(aminocarbonyl)-5-(trifluoromethyl)phenyl]-4-piperidinyl]amino]sulfonyl]-3,5-dichloro- (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 2 HCPLUS COPYRIGHT 2007 ACS on STN

AN 1954:68234 HCPLUS Full-text

DN 48:68234

OREF 48:12172c-f

TI Sulfamide derivatives

IN Hamann, Karl

PA Farbenfabriken Bayer A.-G.

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI DE----876846		19530518	1943DE-F002350	19430601

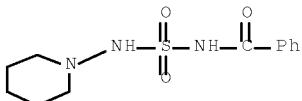
AB SO₂(NH₂)₂ (I) or its N-substituted products containing at least 1 replaceable H atom linked to the N atom are treated with an acylating agent, possibly in the presence of an inert solvent and (or) acid-binding agent, to give sulfamide derivs. useful as intermediates in the manufacture of dyes or remedies. Ac₂O 102 added within 0.5 hr. to I 48 in glacial AcOH 102 parts by weight at 70°, the mixture stirred about 3 hrs. at 70°, and the product which ppts. on cooling filtered and recrystd. from EtOH gives SO₂(NHAc)₂, 70 parts, oblong, colorless needles, m. 153-4°. Similarly are prepared: SO₂(NHCOPr)₂, oblong needles, m. 155-6°, from I and PrCO₂H; H₂NSO₂NHCOPr, oblong needles, m. 143-4°, from I and PrCOCl; H₂NSO₂NHBz, m. 161-2°, from I and BzCl; p-ClC₆H₄COCl; N-cyclohexyl-N'-benzoylsulfamide, 187-8°, from C₆H₁₁NHSO₂NH₂ and BzCl; N-piperidino-N'-benzoylsulfamide, m. 146-7°, from C₅H₁₀NHSO₂NH₂ and BzCl.

IT SSS263-41-1P, Benzamide, N-(piperidinosulfamoyl)-

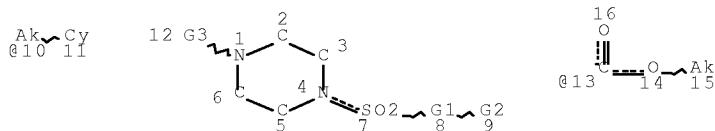
RL: PREP (Preparation)
(preparation of)

RN 855263-41-1 HCPLUS

CN Benzamide, N-(piperidinosulfamoyl)- (5CI) (CA INDEX NAME)



=> d que sta 125
L23 STR



REP G1=(2-3) A
VAR G2=CY/10
VAR G3=CY/13
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

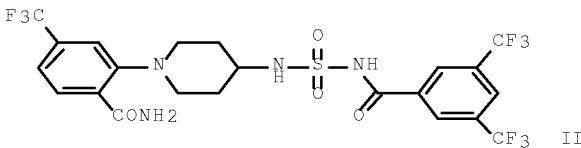
STEREO ATTRIBUTES: NONE
L25 1488 SEA FILE=REGISTRY SSS FUL L23

100.0% PROCESSED 100910 ITERATIONS 1488 ANSWERS
SEARCH TIME: 00.00.02

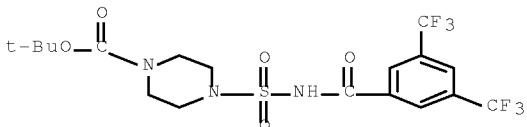
=> d bib abs hitstr 135 tot

L35 ANSWER 1 OF 3 HCPLUS COPYRIGHT 2007 ACS on STN
AN 2003:796680 HCPLUS Full-text
DN 139:307797
TI Preparation of piperazinyl- or piperidinylamine-sulfamic acid amides as
inhibitors of steroid sulfatase
IN Lehr, Philipp
PA Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE
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PI WO2003082842 A1 20031009 2003WO-EP03214 20030327
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

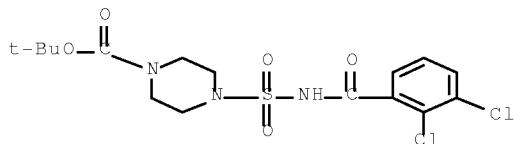
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 HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU,
 LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC,
 SE, SG, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW
 RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE,
 DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE,
 SI, SK, TR
 CA---2480686 A1 20031009 2003CA-2480686 20030327
 AU2003226732 A1 20031013 2003AU-0226732 20030327
 EP---1492782 A1 20050105 2003EP-0745281 20030327
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
 BR2003008795 A 20050118 2003BR-0008795 20030327
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 US2006052393 A1 20060309 2005US-0509259 20050503
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 PRAI 2002GB-0007500 A 20020328
 2002GB-0025679 A 20021104
 2003WO-EP03214 W 20030327
 OS MARPAT 139:307797
 GI



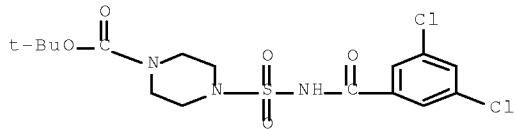
AB The title compds. R1NR2SO2NHCOR3 [I; NR1R2 = piperazino (wherein the second N atom is substituted by alkoxy carbonyl or aryl) ; or R1 = H and R2 = piperidinyl, attached via a carbon atom of the piperidinyl ring (wherein N is substituted by alkoxy carbonyl or aryl); R3 = aryl, arylalkyl], useful for the manufacture of a medicament in diseases mediated by the action of steroid sulfatase, were prepared. E.g., a 5-step synthesis of II (starting from 4-benzylaminopiperidine-1-carboxylic acid tert-Bu ester and sulfamide), was given. The compds. I show activity in the assay of human steroid sulfatase (rel IC50 in the range of 0.0046 to 350). Pharmaceutical composition comprising the compound I is claimed.
 IT 610798-84-0P 610798-86-2P 610798-88-4P
 610798-90-8P 610798-93-1P 610798-94-2P
 610798-95-3P 610798-96-4P 610798-97-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of piperazinyl- or piperidinylamine-sulfamic acid amides as inhibitors of steroid sulfatase)
 RN 610798-84-0 HCPLUS
 CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)benzoyl]amino]sulfonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



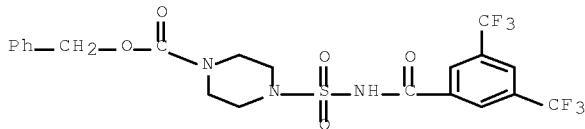
RN 610798-86-2 HCPLUS
 CN 1-Piperazinecarboxylic acid, 4-[[[(2,3-dichlorobenzoyl)amino]sulfonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



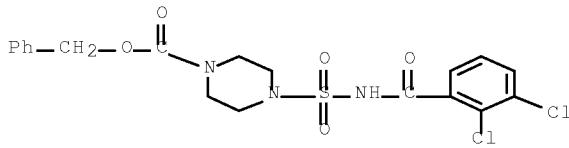
RN 610798-88-4 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-dichlorobenzoyl]amino]sulfonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



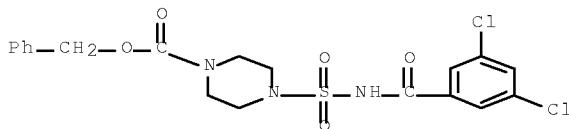
RN 610798-90-8 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-bis(trifluoromethyl)benzoyl]amino]sulfonyl]-, phenylmethyl ester (CA INDEX NAME)



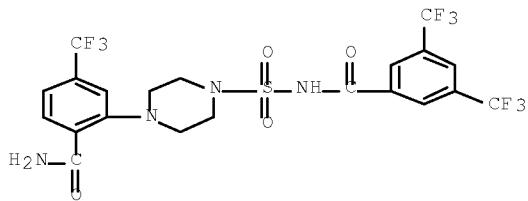
RN 610798-93-1 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[2,3-dichlorobenzoyl]amino]sulfonyl]-, phenylmethyl ester (CA INDEX NAME)



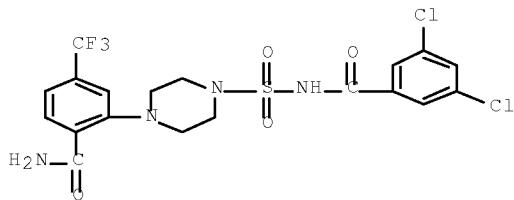
RN 610798-94-2 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[[3,5-dichlorobenzoyl]amino]sulfonyl]-, phenylmethyl ester (CA INDEX NAME)



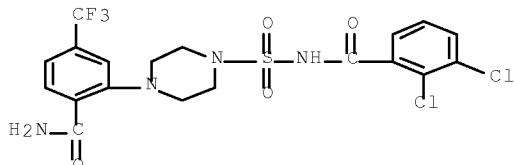
RN 610798-95-3 HCAPLUS
CN Benzamide, N-[[4-[2-(aminocarbonyl)-5-(trifluoromethyl)phenyl]-1-piperazinyl]sulfonyl]-3,5-bis(trifluoromethyl)- (CA INDEX NAME)



RN 610798-96-4 HCAPLUS
 CN Benzamide, N-[(4-[2-(aminocarbonyl)-5-(trifluoromethyl)phenyl]-1-piperazinyl)sulfonyl]-3,5-dichloro- (CA INDEX NAME)

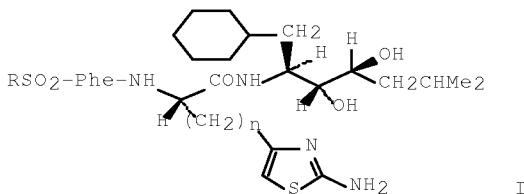


RN 610798-97-5 HCAPLUS
 CN Benzamide, N-[(4-[2-(aminocarbonyl)-5-(trifluoromethyl)phenyl]-1-piperazinyl)sulfonyl]-2,3-dichloro- (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
 AN 1992:490743 HCAPLUS Full-text
 DN 117:90743
 TI Structure-activity relationships of a series of 2-amino-4-thiazole-containing renin inhibitors
 AU Patt, William C.; Hamilton, Harriet W.; Taylor, Michael D.; Ryan, Michael J.; Taylor, David G., Jr.; Connolly, Cleo J. C.; Doherty, Annette M.; Klutckho, Sylvester R.; Sircar, Ila; et al.
 CS Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
 SO Journal of Medicinal Chemistry (1992), 35(14), 2562-72
 CODEN: JMCMAR; ISSN: 0022-2623
 DT Journal
 LA English
 OS CASREACT 117:90743
 GI



I



II

AB A series of renin inhibitors, e.g. I (R = morpholino, piperazino, n = 0-2) and II (R = morpholino, n = 1), was synthesized that contained a 2-amino-4-thiazolyl moiety at the P2 position. These derivs. are potent inhibitors of monkey renin in vitro and are selective in that they only weakly inhibit the closely related aspartic proteinase, bovine cathepsin D. I (R = morpholino, n = 0, 1; R = piperazino, n = 1) and II exhibited oral blood pressure lowering activity in high-renin normotensive monkeys. One of these compds., I (R = morpholino, n = 1) (PD 134672), was selected for further evaluation in renal hypertensive monkeys, on the basis of its superior efficacy and duration of action in the in vitro assays and the normotensive primate model.

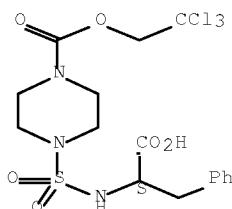
IT 135704-27-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(peptide coupling reactions of, in preparation of renin inhibitors)

RN 135704-27-7 HCPLUS

CN 1-Piperazinecarboxylic acid, 4-[([(1-carboxy-2-phenylethyl)amino]sulfonyl]-, 1-(2,2,2-trichloroethyl) ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L35 ANSWER 3 OF 3 HCPLUS COPYRIGHT 2007 ACS on STN

AN 1991:632884 HCPLUS [Full-text](#)

DN 115:232884

TI Preparation of aminoazole-containing peptide analogs as renin inhibitors and antiretroviral agents

IN Conolly, Cleo; Doherty, Annette Marian; Hamilton, Harriet Wall; Patt, William Chester; Sircar, Ila

PA Warner-Lambert Co., USA

SO Eur. Pat. Appl., 44 pp.

CODEN: EPXXDW

DT Patent

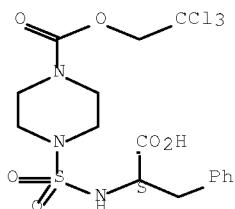
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP----399556	A1	19901128	1990EP-0109990	19900525
	EP----399556	B1	19941228		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US---5238923	A	19930824	1990US-0511271	19900425
	AU---9055908	A	19901129	1990AU-0055908	19900524
	AU---625354	B2	19920709		
	CA---2017552	A1	19901126	1990CA-2017552	19900525
	NO---9002318	A	19901127	1990NO-0002318	19900525
	JP---03086870	A	19910411	1990JP-0134257	19900525
	JP---2980129	B2	19991122		
	ZA---9004043	A	19920129	1990ZA-0004043	19900525

ES---2066905 T3 19950316 1990ES-0109990 19900525
 US---5453488 A 19950926 1993US-0038728 19930326
 US---5643879 A 19970701 1995US-0440585 19950515
 PRAI 1989US-0357561 A 19890526
 1990US-0511271 A 19900425
 1993US-0038728 A3 19930326
 OS MARPAT 115:232884
 GI For diagram(s), see printed CA Issue.
 AB Title compds. [I; A = H, Me3CO2C, PhCH2O2C, Me3CSO2CH2CH(CH2Ph)CO, RR1NSO2, etc.; R, R1 = H, (OH- or amino-substituted) alkyl; B = null, Phe, Tyr, Tyr(OMe); X1 = statine residue (analog); D = null, OH, amino; E = H, alkanoyl, PhCH2O2C, Me3CO2C, C13CCH2O2C; n = 0-2; X, Y = O, S, N, NH; 1 of X, Y must be N], were prepared. Thus, TROC-SPI-Phe-OH (TROC = C13CCH2O2C, SPI = N-piperazinylsulfonyl) (preparation given) in DMF was stirred with DCC and hydroxybenzotriazole at 15° for 30 min; (S)-ATM(TROC)-CAD [ATM = 3-(2'-amino-4'-thiazolyl)alanyl, CAD = Q1] in DMF was added and the mixture was stirred 48 h at room temperature to give a coupling product, which was deprotected with Zn/HOAc/MeOH to give H-SPT-Phe-(S)-ATM-CAD. The latter inhibited remin with IC50 of 0.16 nM.
 IT 135704-27-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for renin inhibitor and antiretroviral peptide)
 RN 135704-27-7 HCPLUS
 CN 1-Piperazinecarboxylic acid, 4-[(1-carboxy-2-phenylethyl)amino]sulfonyl-, 1-(2,2,2-trichloroethyl) ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 09:38:00 ON 06 NOV 2007)

FILE 'REGISTRY' ENTERED AT 09:38:25 ON 06 NOV 2007

L1 STR
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 L3 STR L1
 L4 1 L3
 L5 1 PIPERIDINE/CN
 L6 1217938 46.156.1/RID
 L7 1 L3 SAM SUB=L6
 L8 379 L3 FULL SUB=L6

FILE 'HCPLUS' ENTERED AT 09:46:40 ON 06 NOV 2007

L9 28 L8
 L10 1 US20060052393/PN

FILE 'REGISTRY' ENTERED AT 09:47:41 ON 06 NOV 2007

FILE 'HCPLUS' ENTERED AT 09:47:41 ON 06 NOV 2007
 L11 TRA L10 1- RN : 25 TERMS

FILE 'REGISTRY' ENTERED AT 09:47:41 ON 06 NOV 2007

L12 25 SEA L11
 L13 4 L12 AND L8

FILE 'HCPLUS' ENTERED AT 09:48:38 ON 06 NOV 2007

L14 1 L13

FILE 'HCAOLD' ENTERED AT 09:49:31 ON 06 NOV 2007

L15 1 L9
 SEL HIT RN

FILE 'REGISTRY' ENTERED AT 09:50:01 ON 06 NOV 2007

L16 1 E1-2

L17 FILE 'HCAPLUS' ENTERED AT 09:51:41 ON 06 NOV 2007
18 L9 AND (PD<=20030327 OR AD<=20030327 OR PRD<=20030327)

L18 FILE 'REGISTRY' ENTERED AT 11:12:50 ON 06 NOV 2007
329 E3-331

L19 FILE 'REGISTRY' ENTERED AT 11:32:00 ON 06 NOV 2007
4 L18 AND (C12H17N3O3S OR C20H19CL2F3N4O4S OR C22H19F9N4O4S)

L20 FILE 'HCAPLUS' ENTERED AT 11:32:56 ON 06 NOV 2007
2 L19

L21 FILE 'REGISTRY' ENTERED AT 12:54:42 ON 06 NOV 2007
STR

L22 50 L21

L23 STR L21

L24 27 L23

L25 1488 L23 FULL

L26 9 L25 AND L12

L27 FILE 'HCAPLUS' ENTERED AT 13:01:39 ON 06 NOV 2007
0 L26

L28 FILE 'HCAPLUS' ENTERED AT 13:01:47 ON 06 NOV 2007
1 L26

L29 FILE 'REGISTRY' ENTERED AT 13:02:01 ON 06 NOV 2007
1479 L25 NOT L26

L30 FILE 'HCAPLUS' ENTERED AT 13:02:14 ON 06 NOV 2007
72 L29

L31 45 L30 AND (PD<=20030327 OR AD<=20030327 OR PRD<=20030327)
SEL HIT RN
DEL SEL Y
SEL HIT RN

L32 FILE 'REGISTRY' ENTERED AT 13:03:07 ON 06 NOV 2007
248 E1-248

L33 FILE 'REGISTRY' ENTERED AT 13:18:34 ON 06 NOV 2007
1 L32 AND C16H20CL3N3O6S

L34 FILE 'HCAPLUS' ENTERED AT 13:18:53 ON 06 NOV 2007
2 L33

L35 3 L28, L34

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